ALS SPECTRUM

Advanced Light Source :: Facility Report :: 2008-2009

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What's Inside:

U.S. DEPARTMENT OF ENERGY

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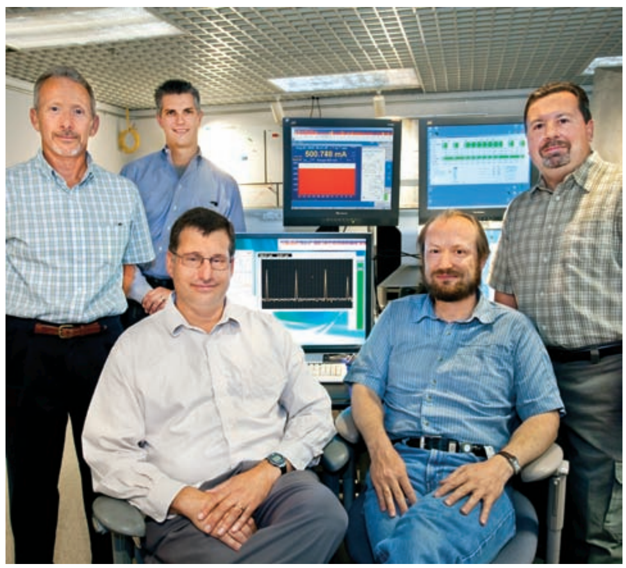
BERKELEY LAB

ALS ADVANCED LIGHT SOURCE

Top-Off: Twice the Light



Key top-off team members gather around a ring-status monitor showing the steady, 500-mA current that doubles the amount of light to ALS users. Counterclockwise: Steve Rossi (project controls), Barry Bailey (head of electrical coordination), David Robin (project leader), Christoph Steier (project manager), and Ken Baptiste (chief engineer, rf and interlocks).

The largest upgrade of the Advanced Light Source since it was originally commissioned in 1993 culminated with the successful transition to top-off user operations on February 11, 2009. The transition was motivated by the possibility of increasing brightness and improving thermal stability, thus keeping the ALS competitive with newer light sources for the next decade.

"It was a terrific feeling," said ALS Director Roger Falcone, "to be able to pull up the ALS ring status on my laptop computer, at any hour of the day, even when I was back at DOE in Washington, and see the high and flat beam current. And then the emails started coming in from the users, highly laudatory and very grateful... We told people at

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Watching Nanoscale Catalysts at Work

Catalysts—substances that speed up chemical reactions without themselves being consumed—are essential players in the interrelated worlds of chemistry, energy, and the environment. Because many catalysts are based on tiny nanometer-sized particles and operate in gaseous atmospheres at high temperature, they could until recently only be observed before and after, but not during, a reaction. In *Science* and *Nature* papers, two research groups, led by Gabor Somorjai of Berkeley Lab and UC Berkeley and Bert Weckhuysen and Frank de Groot of Utrecht University in The Netherlands, independently demonstrated two complementary x-ray approaches to watching nanoscale catalysts at work.

Catalytic systems based on bimetallic particles with controlled size, composition, and structure that are dispersed on high-surface-area supports are widely used in industry, most notably the automobile industry. Owing to the nanoscale size of the particles, the distribution of the two metals composing the particles can shift between surface and

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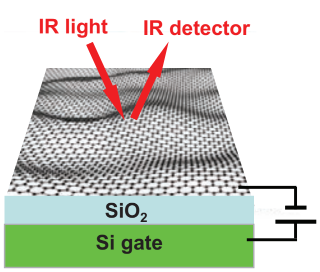
Science Roundup

Infrared View of Graphene

Li et al., *Nature Physics* **4**, 532 (2008)

http://www.als.lbl.gov/als/science/sci_archive/174grapheneIR.html

Graphene—a single layer of carbon atoms arranged in a honeycomb lattice—has very high conductivity that can be tuned by applying a gate voltage. The charge carriers in graphene can travel ballistically over great distances (~1 micron) without scattering. These unusual electronic properties make graphene a promising candidate for future nanoelectronics. Using infrared spectromicroscopy at ALS Beamline 1.4, a group of researchers has succeeded in probing the dynamical properties of the charge carriers in graphene with an accuracy never before achieved. Their results have uncovered signatures of many-body interactions in graphene and have demonstrated the potential of graphene for novel applications in optoelectronics.



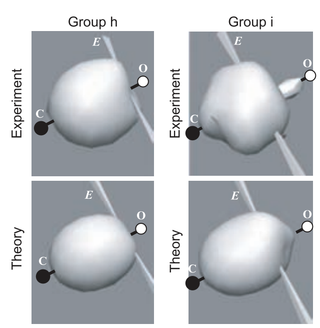
A schematic of the graphene sample integrated in a gate-tunable device. Infrared transmission and reflectance were measured with applied gate voltages.

Auger Measurements in the Molecular Frame

Rolles et al., *Phys. Rev. Lett.* **101**, 263002 (2008)

http://www.als.lbl.gov/als/science/sci_archive/187molecularframe.html

Molecular-frame electron angular distribution (MFAD) measurements provide access to an unprecedented level of detailed information about phenomena involving quantum coherence, such as phases of photoelectron waves, symmetry breaking in molecular dissociation, core-hole localization in molecules, and molecular double-slit interference, all of which are hidden in conventional gas-phase electron spectroscopy, owing to the random orientation of the molecules. While most MFAD studies to date have focused on photoelectrons, a team of scientists from Michigan, the ALS, and Japan has successfully used a novel approach to determine for the first time the MFADs of resonantly excited Auger electrons in carbon monoxide.



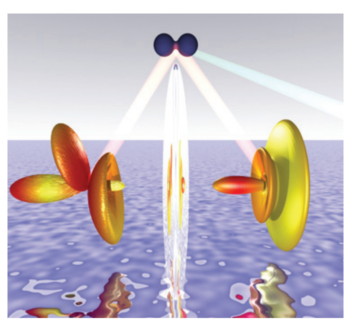
Comparison of three-dimensional MFADs of the h and i groups of the Auger spectrum for carbon monoxide molecules oriented perpendicular to the electric field vector E of the exciting radiation (white sticks) for experiment and theory. The intensity is zero at the intersection of the electric field vector E and the molecular C–O axis.

Core-Hole Localization in N_2

Schöffler et al., *Science* **320**, 920 (2008)

http://www.als.lbl.gov/als/science/sci_archive/177core-holenitrogen.html

The behavior of the core hole created in molecular x-ray photoemission experiments has provided molecular scientists with a valuable window through which to probe the electronic structure and dynamics of molecules. But the answer to one fundamental quantum question—whether the core hole is localized or delocalized—has remained elusive for diatomic molecules in which both atoms are the same element. An international team of scientists from the US and Germany has now resolved the issue with an appropriate twist of quantum fuzziness. By means of coincident detection of the photoelectron ejected from molecular nitrogen and the Auger electron emitted femtoseconds later, the team found that how the measurements are done determines which description—localized or delocalized—is valid.



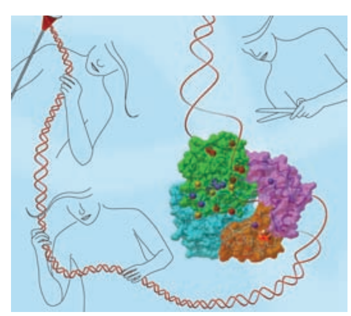
Artist's view of the asymmetric angular distributions obtained by coincident detection of the photoelectron emerging from an N_2 molecule (blue) of the photoelectron (left) and the Auger electron emitted 7 fs later (right) for the case of a localized core hole in an N_2 molecule. As the two electrons form an entangled state, the Auger electron (right) is also localized.

Enzyme's Role in Cancer and Aging

Fan et al., *Cell* **133**, 789 (2008)

http://www.als.lbl.gov/als/science/sci_archive/178xpd.html

XPD helicase is an enzyme that unwinds the DNA double helix; it is one component of a repair mechanism that maintains the integrity of DNA. XPD is unique, however, in that pinpoint mutations of this protein are responsible for three different human diseases: in xeroderma pigmentosum, extreme sensitivity to sunlight promotes cancer; Cockayne syndrome involves stunted growth and premature aging; trichothiodystrophy, characterized by brittle hair and scaly skin, is another form of greatly accelerated aging. At the ALS, researchers recently solved the structure of XPD. The structure gives insight into the processes of aging and cancer by revealing how discrete flaws—as simple as a change in either of two adjacent amino acid residues—can lead to diseases with completely different physical manifestations.



XPD is shown dividing DNA that is held by the three fates of Greek mythology: Clotho (left) spun the thread of life, Lachesis (bottom) measured it, and Atropos (right) cut the thread, determining life span. XPD opens damaged DNA to allow repair enzymes to excise the damaged patch. Figure design by Doug Ng and Michael Pique.

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Read more about these and other science highlights at http://www-als.lbl.gov/als/science/

Self-Assembly of Polymer Nano-Elements

Park et al., *Science* **323**, 1030 (2009)

http://www.als.lbl.gov/als/science/sci_archive/182copolymers.html

Self-assembly of polymers promises to vastly improve the properties and manufacture of nanostructured materials, since self-assembly is highly parallel, versatile, and easy. Especially promising are novel compounds known as block copolymers, formed by two different polymers linked together. Patterned arrays have been produced using lithographic techniques, but those methods are painstaking and have yet to produce perfect surfaces over large areas. Recently, a group of researchers used faceted surfaces of commercially available sapphire wafers to guide the self-assembly of block copolymers. Grazing-incidence small-angle x-ray scattering at the ALS verified the arrays' quasi long-range order over large wafer surfaces. It's expected that this new method will revolutionize the microelectronic and storage industries and perhaps others, such as photovoltaics.

Fertilizing the Ocean with Iron

Toner et al., *Nature Geoscience* **2**, 197 (2009)

http://www.als.lbl.gov/als/science/sci_archive/183ocean-iron.html

Despite the considerable amount of iron entering the oceans from the continents and from hydrothermal vents, there are large regions where iron availability is so low that it limits life. Oceanographers have explained this by assuming that the iron in the sea is primarily incorporated as Fe(III) into minerals lacking the mobility to circulate and unavailable to sea life as a nutrient. Now, a collaboration led by researchers from the Woods Hole Oceanographic Institution has reported that the hydrothermal plumes emerging from the vents actually contain iron in both Fe(II) and Fe(III) oxidation states associated with organic material from nearby flora and fauna. The work suggests that the organic matrices prevent oxidation and precipitation of the Fe(II), perhaps increasing both its circulation through the world's oceans and its bioavailability as a deep-sea nutrient.

Ebolavirus Structure with Survivor Antibody

Lee et al., *Nature* **454**, 177 (2008)

http://www.als.lbl.gov/als/science/sci_archive/175ebola.html

Ebolavirus causes severe hemorrhagic fever with 50–90% mortality. No vaccines or treatments are yet available, and its frequent re-emergence, high prevalence among wildlife, and ease of importation make it a significant public health concern. A team of researchers from the Scripps Research Institute has determined the structure of a glycoprotein from the viral surface in complex with a rare antibody from a human survivor. This work explains how the glycoprotein (GP) mediates recognition of the host cell, drives fusion of the viral and host membranes, and masks itself from immune surveillance. The structure also explains why antibodies that neutralize the virus are so rare, identifies the very few sites to which a neutralizing antibody might bind, and thus, provides templates for vaccines and antibodies against the virus.

Domain-Wall Pinning and Magnetic Vortices

Vansteenkiste et al., *Phys. Rev. B* **77**, 144420 (2008)

http://www.als.lbl.gov/als/science/sci_archive/172vortices.html

Soft magnetic, micron-sized thin-film structures with magnetic vortices are intriguing systems that may one day be used in ultrafast computer memories. In such systems, the otherwise in-plane magnetization turns perpendicular to the plane at the center of the vortex, forming the vortex core. Because such a core has two possible polarizations (up or down) and can be switched between these two states by a small alter-

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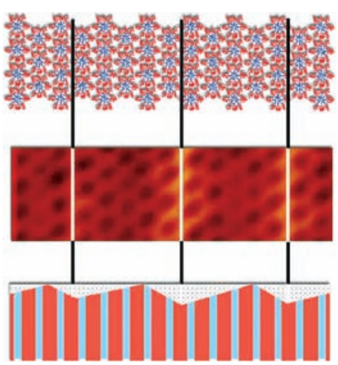
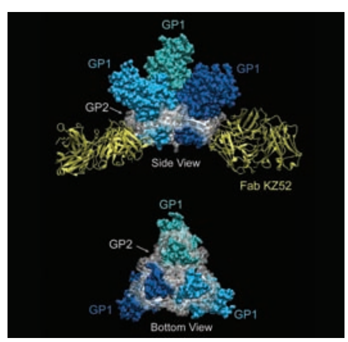
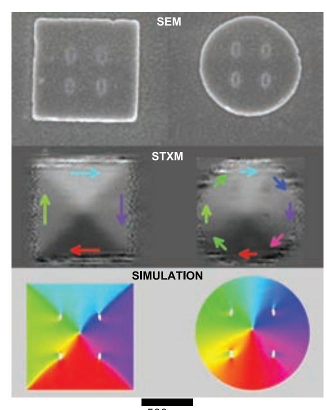


An overhead view (top) of block-coploymer structures. An atomic-force microscope image (center) shows the densely packed cylinders, dark in the center. The side view diagram (bottom) shows how the cylinders arrange themselves along the ridges of the crystalline facets.

Fluids from hydrothermal vents, such as the Tica vent shown here, contain about one million times more iron than regular ocean water. While it was thought that the iron pumped out immediately forms mineralized particles when it mixes with seawater, it has now been found that some of the iron remains in a form that is bioavailable to organisms in the ocean. (Photo: Olivier Rouxel © Woods Hole Oceanographic Institution)



The crystal structure of *Ebolavirus* GP reveals a three-lobed chalice-like structure. The three GP1 subunits (colored blue and green), mediate attachment to new host cells and are tethered together by the three GP2 subunits (white). The human antibody KZ52 (yellow) binds the GP at the base of the chalice, where it bridges GP1 to GP2, before fusion of the membranes.



Top: SEM images of square- and disk-shaped structures. Center: Corresponding STXM images showing the x-component of the magnetization (the arrows also indicate the direction of the magnetization). Bottom: Micromagnetic simulation of the magnetization in these structures.

Top-Off Success

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DOE we were capable of doing it; we did it. We told our users we could do it, and we did it."

The top-off operational mode allows frequent injection of electron beam into the storage ring, resulting in a nearly constant current. This mode presents several large advantages for users. Instead of having multiple injections of a large number of electrons in a short time period followed by uninterrupted beam decay over the course of eight hours, a small number of electrons is added to the storage ring at approximately every 30 to 60 seconds. The constant beam current enhances the flux and brightness of the radiation while simultaneously improving the thermal stability of the machine and its beamlines.

According to David Robin, ALS Division Deputy for Operations and Accelerator Development, top-off is exceeding expectations, with less of a "teething period" than anticipated. As expected, he said, we have improved thermal stability, we increased the flux, and we've increased the usable beam time. Furthermore, reliability has actually improved: we're getting close to our best operation since the ALS was commissioned.

In April, the ALS ramped up to its target of 500 mA of average storage-ring current. The higher average current level in the storage ring translates into a 100% increase in photon flux. Also, the process of slowly decreasing the vertical emittance has begun. Later in the year, the vertical emittance was reduced in user operations, increasing the brightness by up to an additional factor of four. This corresponds to a reduction of electron beamsize and divergence to about half their previous values. So, overall, the upgrade increased the flux by a factor of two and the brightness by a factor of up to eight. The installation of newer insertion devices with smaller gaps will provide additional gains in the future.

In terms of stability, it is estimated that by eliminating the current dependence of beam-position monitors and by reducing the thermal motion of magnets, girders, etc., the medium-term orbit drift has been reduced by a factor of two to three. On top of that, user beamlines profit from the steady heat load that no longer introduces thermal drifts in beamline components. Finally, it is of advantage to many users that they do not need to normalize their measurement data to their incoming photon flux anymore. This makes measurements easier and reduces noise and systematic errors. Responses from users, who have anxiously anticipated top-off operation for several years, have been uniformly positive.

Similar to the superbend upgrade in 2001, the transition to top-off mode was a major surgery, with a lot of risks and breaking new ground in many areas. For example, bunch cleaning for two-bunch mode was a requirement for which there was no solution when the project began. The method ultimately devised by the team proved to work extremely well, resulting in greater bunch purity than before and an increase in average two-bunch current by nearly a factor

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Science Roundup

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nating magnetic field, it could serve as a memory bit in future magnetic memory devices. However, these magnetic structures often contain numerous imperfections such as domain-wall pinning sites, which have to be taken into account for the practical application of such systems. To study how these defects affect the dynamics of magnetic vortices, researchers from Belgium, Germany, and the United States investigated square- and disk-shaped thin-film structures with artificially introduced imperfections in the form of nanometer-sized holes. They used time-resolved STXM at ALS Beamline 11.0.2 to determine the frequency at which these vortices vibrate (their eigenfrequency). The imperfections were found to cause a higher vibrational frequency in square-shaped structures, but did not influence the disk-shaped structures. Knowledge of the frequency is crucial for vortex-based memories, since the electric signal for writing data needs to be precisely tuned to it.

A New Form of Macroscopic Quantum Weirdness

Hsieh et al., *Science* **323**, 919 (2009)

http://www.als.lbl.gov/als/science/sci_archive/184insulators.html

It has recently been proposed that insulators with large band gaps and strong spin-orbit coupling can host a new phase of quantum matter called a topological insulator that is characterized by entangled wavefunctions. The proposal has now been realized by an international collaboration led by researchers from Princeton Univer-

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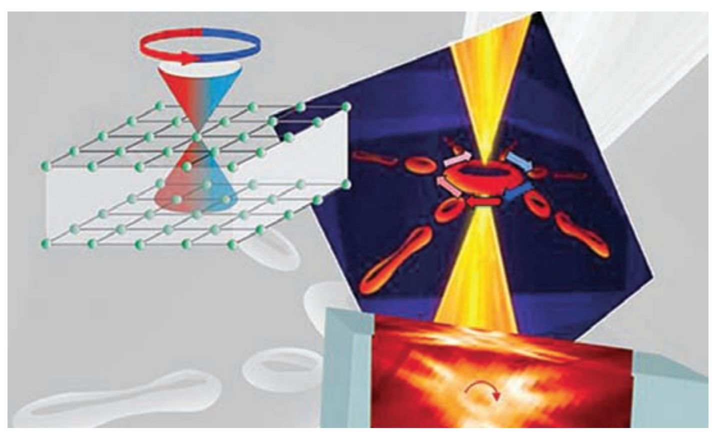

A new type of quantum matter called a topological insulator contains only half an electron pair (represented by just one cone in schematic crystal structure at top left), which is observed in the form of a single ring (red) in the center of the electron-map (top right) with electron spin in only one direction. This highly unusual observation shows that if an electron is tagged "red" and then undergoes a full 360-degree revolution about the ring, it does not recover its initial face as an ordinary everyday object would, but instead acquires a different color "blue" (represented by the changing color of the arrows around the ring). This new quantum effect can be the basis for the realization of a rare quantum phase that had been a long-sought key ingredient for developing quantum computers that can correct themselves.

Catalysts at Work

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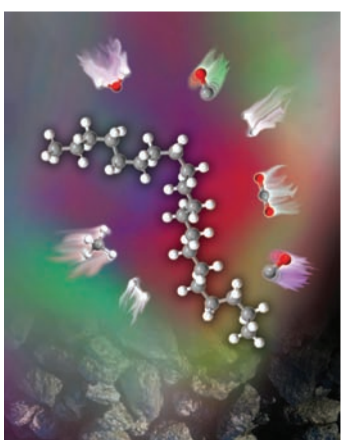
interior during the catalysis process—shifts that can dramatically affect catalyst activity and selectivity—but exactly how has not been known.

The Somorjai group turned to x-ray photoemission spectroscopy on ALS Beamline 9.3.2, where there is a unique ambient-pressure photoemission chamber that allows measurements under reaction conditions. The group prepared model catalysts consisting of $Rh_{0.5}Pd0._5$ and $Pt_{0.5}Pd_{0.5}$ nanoparticles arrayed on silicon wafers. Spectra from a series of photon energies yielded depth profiles of the particle composition and chemical state. The profiles roughly corresponded to a surface shell, usually the catalytically active area, surrounding an interior core [Tao et al., *Science* **322**, 932 (2008)].

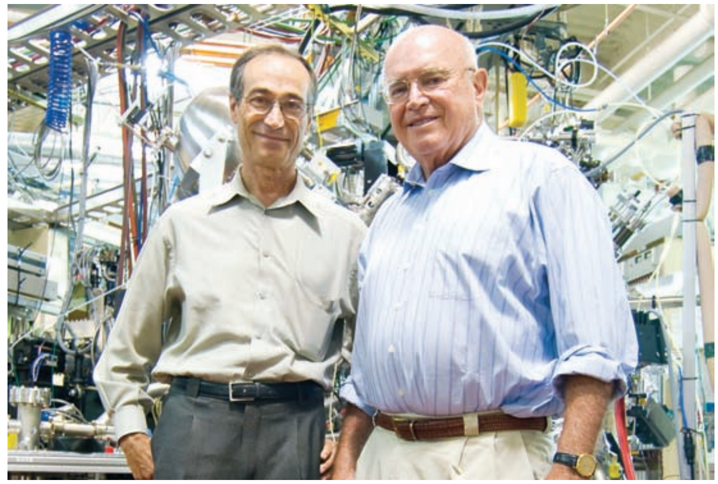
Cycling the samples through a sequence of oxidizing, catalytic, and reducing conditions, the group found that the as-prepared $Rh_{0.5}Pd_{0.5}$ nanoparticles had rhodium-rich shells and $Pt_{0.5}Pd_{0.5}$ nanoparticles had palladium-rich shells. Thereafter, the composition of the shell and the core-shell distribution of the $Rh_{0.5}Pd_{0.5}$ nanoparticles changed dramatically but reversibly in response to changes in the reactant gas composition, whereas no substantial composition shifts occurred in the $Pt_{0.5}Pd_{0.5}$ nanoparticles.

While nanoscale metal or metal oxide particles dispersed on high-surface-area supports are the active elements of most industrial catalysts, their overall performance depends not only on their size and composition but also on their multiple interactions with the support, reactants, and products. The Fischer-Tropsch synthesis involved in producing high-purity chemicals and transportation fuels from sources other than crude oil is a case in point. The complex chemistry associated with the iron-based catalyst has made even the identity of the active catalyst at work an unsolved mystery.

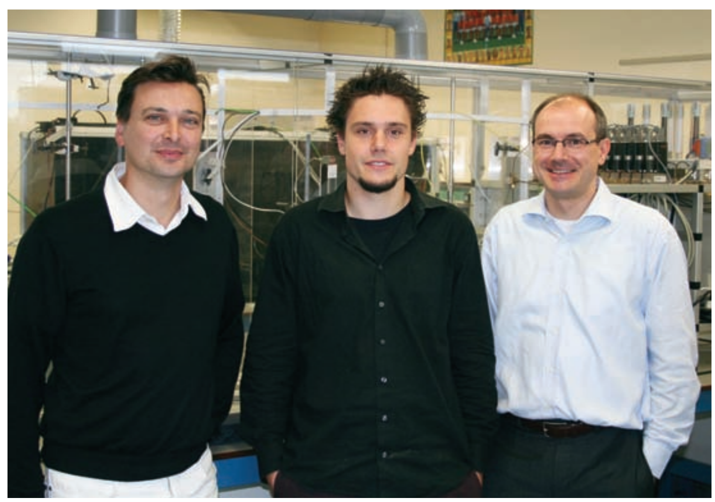
The de Groot–Weckhuysen group combined scanning transmission x-ray microscopy (STXM) at ALS Beamline 11.0.2 with a reaction chamber adapted from electron microscopy to identify the chemical species present for an iron-based Fischer–Tropsch synthesis catalyst under working conditions and to image their distribution on the nanoscale. For its in-situ study, the Dutch team used a catalyst consisting of an iron oxide phase dispersed on silicon oxide (SiO_2) [de Smit et al., *Nature* **456**, 222 (2008)].



In the Fischer-Tropsch synthesis reaction, a carbon–hydrogen chain molecule is generated from synthesis gas (CO and H_2) with the help of a catalyst comprising an iron oxide phase dispersed on silicon oxide (SiO_2) with water and carbon dioxide as by-products. In the drawing, carbon is gray, hydrogen is white, and oxygen is red.



Miquel Salmeron and Gabor Somorjai at ALS Beamline 9.3.2.



Frank M.F. de Groot, Emiel de Smit, and Bert M. Weckhuysen in their laboratory at Utrecht University, The Netherlands.

Measurements in reducing and catalytic atmospheres at high temperature with a spatial resolution of 40 nm generated chemical contour maps for the species present. Quantitative analysis of the spectra yielded calculated proportions for the various phases present at each point. These measurements demonstrated that STXM can provide details about the morphology and composition of complex catalytic system under realistic conditions.

The new windows opened by these two groups could provide the insight needed to guide the design of cheaper and smarter catalysts that are fine-tuned for today's energy and environmental challenges, such as reactions that sweep toxins from pollutants, feed hydrogen fuel cells, and drive fuel-refinement techniques. Ultimately, "smart" catalysts whose structures change advantageously depending on the reaction environment may be possible. ■

THE RING AROUND THE RING AROUND THE RING

Experimental Systems Group: Focus on X Rays

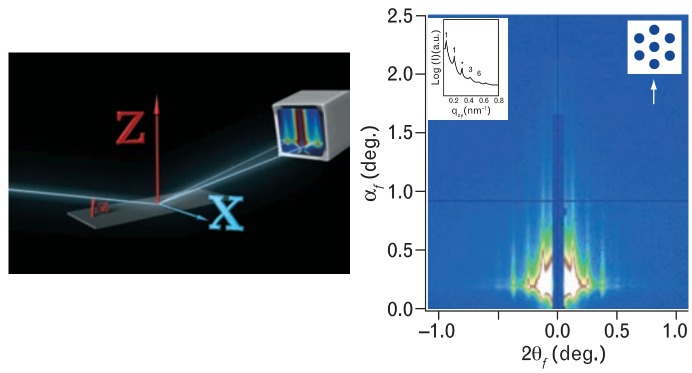
by Howard Padmore

The ALS has developed over the years a complementary portfolio of infrared, VUV, soft x-ray, medium-energy, and hard x-ray beamlines. The hard x-ray techniques are focused on the DOE's energy mission—advancing our understanding, for example, of polymer chemistry and physics related to plastic electronics and solar cells, interfaces in batteries, the properties of new lightweight composite materials, and the structure of new catalysts. In the lifecycle of a beamline, there is a long stretch of time after initial operation in which performance can be steadily improved, often by orders of magnitude, by use of new technologies. Here we report on a few of these developments that are emblematic of the advances that are constantly made.

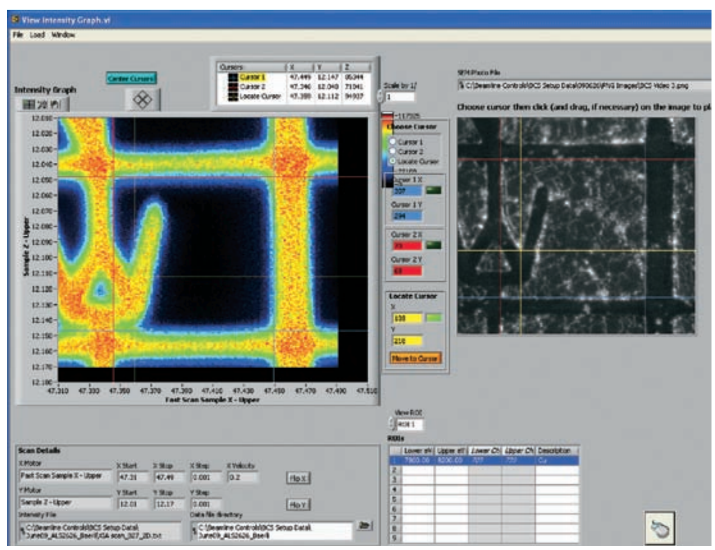
Beamline 7.3.3 is dedicated to small- and wide-angle x-ray scattering (SAXS-WAXS). This technique allows one to determine information about the structure of noncrystalline or quasi-crystalline samples, useful in studying protein assembly, phase transformations in polymers, and superstructure organization in liquid crystals. Its use, however, is restricted to bulk materials. On Beamline 7.3.3, a team led by Alex Hexemer has implemented grazing-incidence (GI) SAXS, which uses reflection geometry to study near-surface regions. As many polymer applications now involve thin-film technology, the ability to probe the near surface is very important.

One of the first applications was to probe long-range order in very thin layers of self-assembled block copolymer (BCP) films. The Russell group (U. Mass. Amherst) in this case is developing BCP films as addressable templates, and so their focus is to perfect the ordering of the films over as large a scale as possible. GI-SAXS is proving to be an ideal tool for measuring the degree of structural perfection. Another advance has been the implementation of a small pixel detector that greatly improves sensitivity and speed compared to existing CCD-based detectors. Other advances include development of low-scatter slits and windows and the use of stop-flow devices to optimize our ability to measure the structure of proteins in solution and as they assemble and undergo conformational changes.

Electronic and mechanical properties of materials do not only depend on the properties of the constituents, but also on the interplay between various components. Measuring properties on the inter- and intra-grain level is thus important for the design of composite devices. Beamline 12.3.2 specializes in measuring chemical and mechanical properties of materials with high spatial resolution using single-crystal Laue diffraction [Kunz et al., *Rev. Sci. Instrum.* **80**, 035108 (2009)]. With this technique, we can map on a submicron scale the distribution of elements, the size of individual grains, and their orientation as well as strains imposed on the grains by internal or external forces. Materials investigated include high-efficiency batteries, solar-cell solder joints, soil samples from mine drainage, and microelectronic devices.



Geometry of GI-SAXS and diffraction pattern from a PS-PEO film [Park et al., *Science* 323, 1030 (2009)].



A fast XRF scanning mode combined with a correlation option allows positioning of the beam on microcrystals even if they are invisible to XRF.

To target the micro-focused x-ray beam on specific regions of interest, the sample has to be positioned very accurately. This requires an easy and accurate correlation between x-ray signals and visual images. We have combined sophisticated two-plane high-numerical-aperture optical viewing, with use of the x-ray fluorescence (XRF) signal generated by the beam, correlating specific markers on the sample with an XRF map. This requires fast and efficient XRF mapping. In cases where the actual region of interest is invisible to XRF, a rapid and reliable extrapolation from XRF markers

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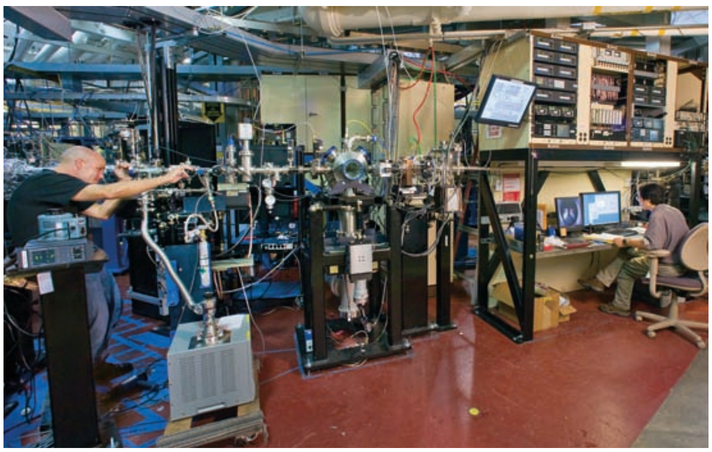
Scientific Support Group: New and Improved Beamlines Enable New Science

by Zahid Hussain, Mike Martin, and Eli Rotenberg



Engineer Nicholas Kelez and beamline scientist Yi-De Chuang work at the new MERLIN beamline in Sector 4.

New Beamlines and Capabilities. Beamline 4.0.3, also known as the Milli-Electron-volt Resolution beamLINe (MERLIN) has taken first light and is undergoing commissioning and initial spectral resolution tests. The beamline features the first quasiperiodic undulator at the ALS, and will achieve the ultimate resolution for angle-resolved photoemission spectroscopy (ARPES) and inelastic scattering.

MAESTRO, the Microscopic and Electronics Structure Observatory, has been awarded funding under the DOE's Single Investigator Small Group Research (SISGR) program. It will replace the existing photoemission branchlines at Beamline 7.0 and feature a new, dedicated half-length insertion device capable of full polarization control above 60 eV and a new entrance-slitless monochromator capable of 3-meV resolution from 20 to 100 eV with extended operation up to 1000 eV.

The new infrared Beamline 5.4, dedicated to environmental, biological, and ultrahigh-resolution studies with mid- and far-infrared light, is nearing completion with commissioning expected to begin in early FY10. The new beamline will collect double the light of the existing infrared beamline and is expected to have endstations with complementary capabilities.

Novel dichroism experiments performed with the eight-pole electromagnet developed at the ALS providing fields up to 0.8 T in arbitrary directions have given us a first glimpse of the wealth of new information contained in XMLD and XMCD angular dependence. A superconducting eight-pole magnet providing magnetic fields of up

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Environmental and Magnetic Studies at 11.0.2

by Hendrik Bluhm, Mary K. Gilles, Tolek Tyliszczak, and David K. Shuh

Between the scanning transmission x-ray microscope (STXM) and ambient-pressure photoelectron spectrometer (APPES), Beamline 11.0.2 continues to be the most oversubscribed beamline at the ALS. STXM experiments are roughly split into those probing environmental materials (soils, catalysis, stardust, actinides, and atmospheric aerosols) and studies probing the magnetic properties of materials. APPES endstation experiments focus on environmental applications and catalysis as well as several new energy-related experiments (batteries and fuel cells). These spectroscopic and microscopic experiments in the soft x-ray region are excellent tools for probing samples under realistic conditions, i.e., with water or water vapor present at ambient temperature.

Recent scientific studies on the APPES endstation explored the Br^- enhancement at the liquid/vapor interface of an aqueous NaCl solution doped with bromide. This system serves as a model system for sea-salt chemistry, as the chemistry of bromine species are associated with sea-salt ice and aerosols and may be involved in ozone depletion episodes during Arctic sunrise. Using the APPES, a crystal of NaCl (doped with NaBr) is cooled in the presence of water vapor until a solution is observed. Comparing the XPS spectra of the solid crystal to that of the solution/vapor interface, an interfacial enhancement of Br^- relative to Cl^- and Na^+, as well as to its bulk concentration, is observed. These results are consistent with simulations. Experimental results indicated that for a saturated solution (in equilibrium with the solid salt), Br^- enhancement at the liquid/vapor interface arises from both the enrichment of Br^- in the solution

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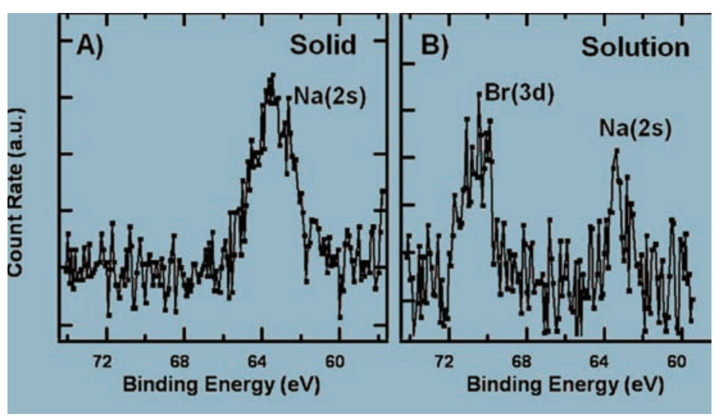

Ambient-pressure XPS spectra of a 0.1% bromide-doped NaCl single-crystal surface (a) under dry (~5% relative humidity) conditions and (b) with the formation of a solution. The Br(3d) and Na(2s) regions are shown [Ghosal et al., *J. Phys. Chem. A* 112, 12378 (2008)].

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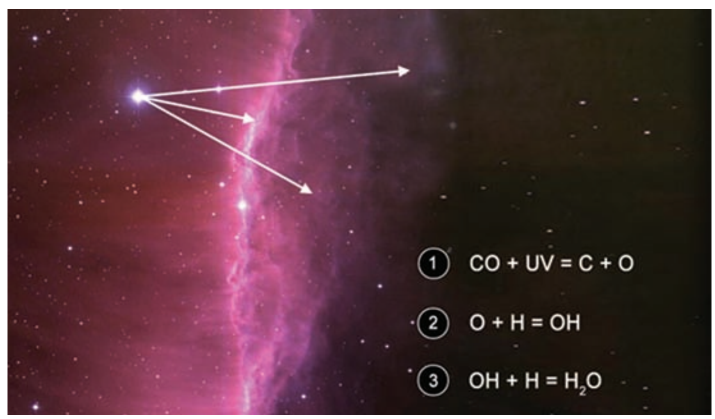
Organic Droplet Reactivity and Cosmochemistry at 9.0.2

by Musa Ahmed

The Chemical Dynamics Beamline 9.0.2 is devoted to the study of fundamental chemical processes using vacuum ultraviolet light. Several endstations support experiments in photoionization spectroscopy, ion and electron imaging, flame studies, clusters, photofragmentation, helium droplet spectroscopy, radical production, aerosol chemistry, nanoparticle physics and chemical imaging. Two examples of the science performed there include a study of the heterogeneous chemistry of organic aerosols [Smith et al., *Atmos. Chem. Phys.* **9**, 3209 (2009)] and a test of the CO self-shielding hypothesis as applied to solar origins [Chakraborty et al., *Science* **321**, 1328 (2008)].

The heterogeneous reactivity of small radicals such as OH at the surface of organic particles or droplets has important implications for the combustion and auto-oxidation of fuel sprays, the formation and destruction of aerosols in the atmosphere, and the chemical aging of soot in urban environments. The heterogeneous reaction of OH radicals with submicron squalane ($C_{30}H_{62}$) particles in the presence of O_2 is used as a model system to explore the reaction rate and oxidation mechanisms that control the chemical transformation of the particle produced after a surface reaction. Detailed kinetic measurements combined with elemental mass spectrometric analysis revealed that the reaction proceeds sequentially by adding an average of one oxygenated functional group per reactive loss of squalane. Based on a comparison between the measured particle mass and model predictions, it appears that significant volatilization of a reduced organic particle would be extremely slow in the real atmosphere. However, as the droplets become more oxygenated, volatilization becomes a significant loss channel for organic material in the particle phase. Together, these results provide a chemical framework in which to understand how heterogeneous chemistry transforms the physiochemical properties of particle-phase organic matter exposed to small gas-phase free radicals.

The concept of isotopic self-shielding in the solar nebula of O_2 and CO has been invoked to explain the enhanced ^{13}C and ^{18}O signatures observed by radio astronomers at the edges of interstellar molecular clouds. Recently, self-shielding of CO has been revitalized to account for the source of isotopically anomalous oxygen in the solar reservoir and as a mechanism for production of meteoritic (refractory minerals) oxygen isotopic compositions. Experiments at the Chemical Dynamics beamline tested the self-shielding hypothesis and found a large oxygen isotopic fractionation during CO dissociation and no apparent evidence of self-shielding. The experiments underscore the critical need for laboratory experiments directed towards resolution of the isotopic anomalies. Models are limited by the lack of experimental observations and these results pave a way for future experiments with relevance to cosmochemistry. ■



Self-shielding has been observed in molecular clouds. Whether or not self-shielding was involved in creating the oxygen isotope ratios in the early solar nebula, the ratios are preserved as the oxygen dissociation products of CO that combine with hydrogen to form hydroxyl radicals and then water, which later reacts with dust grains to form minerals.

XM-2: High-Resolution Tomography of Cells

by Gerry McDermott

During the past year XM-2, a new biological soft x-ray transmission microscope, came online and is accepting external users. Designed and operated by the National Center for X-Ray Tomography (NCXT), the new microscope is producing an unprecedented number of high-resolution, three-dimensional tomograms of biological cells. Each projection image only requires an exposure of 150 ms. As a result, it takes less than three minutes to collect full, 50-nm isotropic resolution tomographic data. The relatively large field of view on XM-2 means that in many cases more than one cell is imaged per experiment. For bacteria and yeast, this can vary from a handful to upwards of one hundred cells being imaged. Consequently, in the last few months, 12 research groups—from as far afield as England, Korea, and Australia—have used XM-2 to tomographically image more than 2,000 cells. Compared to electron microscopy, where obtaining data to reconstruct a tomogram of a single yeast cell is considered a herculean achievement, this is a remarkable step forward in biological imaging, and soft x-ray tomography is therefore now in great demand.

In addition to x-ray imaging, the NCXT team has also broken through an existing barrier in light microscopy. Fluorescence imaging is arguably one

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XM-2 Microscope

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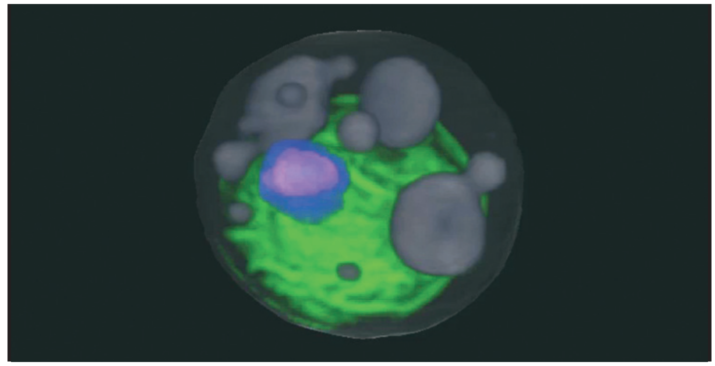
of the most informative and widely used techniques in the biological sciences. It can be used to determine the location of tagged molecules in a living cell and how the relative locations change during the cell cycle as a consequence of disease or in response to environmental factors. Correlation of this information with structural information, such as that produced by soft x-ray tomography, has been a long-standing ambition. To make this a reality, Mark Le Gros and colleagues developed correlated high-aperture cryogenic light microscopy. This instrument allows cells to be flash frozen, imaged using light and, ultimately, x rays. Since this is done in the same instrument, data from the two imaging modalities can be superimposed with relative ease. This development has generated a unique facility at the ALS, and one that is now being used to address key questions in fields as diverse as bioenergy research, drug discovery, and fundamental biology.

For further information on NCXT and XM-2, visit *http://ncxt.lbl.gov*, or contact Carolyn Larabell (calarabell@ucsf.edu). ■



Soft x-ray tomographic reconstruction of an algal cell that has been engineered to produce biofuel (shown in dark gray). In this 50-nm-resolution image, the photosynthetic membranes are shown in green, the nucleus in blue and the nucleolus in pink. This work was carried out in collaboration with Blake Simmons and Seema Singh of the Joint BioEnergy Institute (JEBI).

Crystallography: Rise of Automation and Remote Data Collection

by Paul Adams

The Howard Hughes Medical Institute beamlines are entering the final stages of a $4.8M upgrade project. Beamlines 8.2.1 and 8.2.2 have now finished installing and commissioning the ACTOR sample automounters. Both beamlines are now fully remote capable, which means that users are able control sample mounting, data collection and analysis from their home labs. This has dramatically increased the efficiency of data collection and significantly reduced the cost of protein crystallography experiments, since users no longer have to travel to the synchrotron.

To facilitate studies on small crystals, a microdiffractometer was installed at Beamline 8.2.1. The new equipment allows precise sample positioning to within 2 microns, excellent sample viewing of very small crystals, and an off-axis crystal positioning stage. As part of the beamline optics upgrades, a new toroidal focusing mirror was purchased and installed in Beamline 8.2.1, and new parabolic mirrors have been ordered and are currently being polished. The new optics will increase brightness by a factor of 4 to 5 and decrease spot size to 30 microns, greatly facilitating structure solution on large macromolecular complexes.

The past year has seen a dramatic rise in the adoption of automated sample handling and remote data collection amongst macromolecular crystallography users. This rise has primarily been driven by significant recent enhancements to the beamline hardware and the deployment of new and improved remote-access technologies. In Sector 5, improvements to the existing Berkeley Automounter sample-handling system have dramatically improved both its reliability and its total capacity while in Sector 8, the installation of the Rigaku automounter systems have introduced this capability for the first time. This increased adoption of automated sample handling by users culminated at the end of July with 100% utlization across all Berkeley Center for Structural Biology (BCSB) beamlines for the first time.

Sample viewing using the MD2 microdiffractometer at Beamline 8.2.1; circle is 100 microns in diameter.

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Scientific Support Group

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to 6 T in arbitrary directions has recently been funded with $1.5M through the American Recovery and Reinvestment Act (ARRA). The endstation will allow the performance of this new class of soft x-ray dichroism experiments on a wide variety of complex oxides, dilute magnetic semiconductors, as well as engineered magnetic nanostructures, leading to fundamentally new insights into their magnetic and electronic structure.

The ambient-pressure XPS (AP-XPS) technique, which was first pioneered at the ALS, has produced many important results (see "Watching Nanoscale Catalysts at Work"). A new ambient-pressure photoemission endstation at Beamline 9.3.2 is currently being commissioned and will be available for general users at the start of FY10. The new endstation, designed in a collaboration between VG Scienta and the ALS, has 10 times more efficient electron collection than the original endstation. New features include one-dimensional imaging capability with a spatial resolution better than 50 microns and angle-resolved photoemission capability with a pressure up to 1–2 mbar and temperature up to 1000 K.

A novel time-of-flight analyzer for spin-ARPES experiments has been developed and has achieved an energy resolution of its target value of 10 meV through a 90-degree band-pass filter. This analyzer employs a time-of-flight analyzer (10 times more efficient than dispersive analyzers) coupled to a high-efficiency exchange scattering spin detector (about 50–100 times more efficient for spin detection than Mott detectors).

The experimental capabilities of the Electronic Structure Factory at Beamline 7.0.1.2 continues to make big strides; notable for this year is the successful implementation of a pulse laser deposition system that is allowing in-situ electronic structure measurements of samples that cannot be cleaved and studied otherwise with ARPES.

Beamline 12.0.1 has taken delivery of the latest generation of electron spectrometer, the R3000 from Gammadata/Scienta. This instrument will provide nearly three times the angular window for data collection and up to twice the energy resolution as the previous SES-100. This will speed up and improve the data collection on this heavily oversubscribed beamline. A new experimental ARPES chamber housing the R3000 analyzer is being commissioned and will be available to users in FY10. The old SES-100 will be coupled with a helium lamp to allow users preliminary exploratory experiments prior to studying their samples at the beamline, again increasing efficiency and maximizing beamtime

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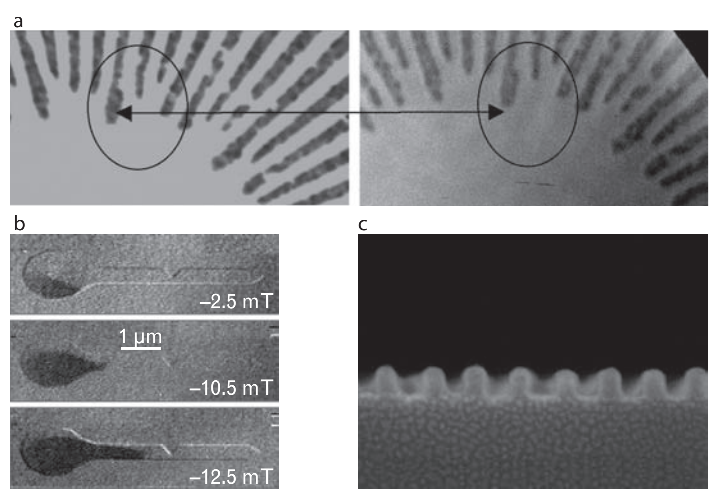
CXRO: High-Performance Tools for Nanoscience Research

by Erik Anderson

The Center for X-Ray Optics (CXRO) has made significant progress both scientifically and technologically in its x-ray imaging, metrology, and industry-funded EUV lithography research programs. The leading research performed at the center's nanofabrication and coating facilities enables it to provide high-resolution diffractive optics, coatings, and other nanostructures, for its own activities and for the support of numerous ALS activities.

The full-field soft x-ray microscope, XM-1, at Beamline 6.1.2 is a unique and highly demanded analytical tool for nanoscience research, combining excellent spatial (12-nm) and temporal (70-ps) resolution with a rich set of contrast mechanisms: elemental, chemical, topological, and magnetic. Using a new resist process, 12-nm zone plates have been fabricated and tested, reaching a new milestone of resolving 12-nm lines and spaces. Figure (a) shows a scanning transmission electron micrograph (STEM) and the corresponding soft x-ray microscopy image of a test sample.

Magnetism research using this microscope is focusing on a fundamental understanding of magnetic properties at nanometer scales—properties that are important to novel concepts of



(a) STEM (left) and soft x-ray (right) micrograph of a gold test object demonstrates 12-nm spatial resolution. (b) Magnetic soft x-ray microscopy of field-driven domain-wall propagation along a ferromagnetic notched nanowire as function of applied field. (c) 22-nm spatial resolution patterning with a high-sensitivity EUV resist.

high-density and high-speed magnetic storage media. The dynamics of a magnetic domain wall (DW) in confined geometries after excitation by short spin-current pulses was analyzed from time-resolved x-ray images

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Scientific Support Group

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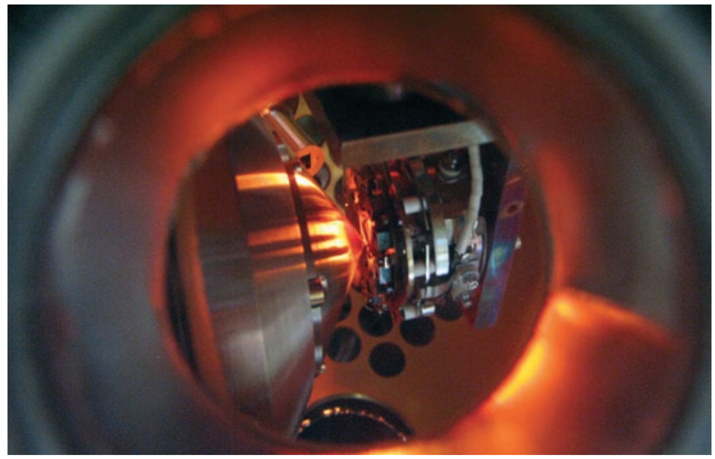
effectiveness for our users.

The Beamline 12.0.2.2 coherent scattering science endstation recently had a sample stage upgrade to state-of-the-art nanopositioning devices known as "attocubes." This upgrade allows reliable and facile insertion of three pinhole arrays into the x-ray beam. The x- and y-stages now have a precession of 50 and 200 nm, respectively, and significantly improved stability and reduced drift.

Soft x-ray magnetic dichroism spectroscopy helps our understanding of complex heteromagnetic nanostructures via element-, valence-, and site-specific magnetic information with high sensitivity and tunable probing depth. The new 2-T magnet endstation at ALS bend-magnet Beamline 6.3.1, funded jointly by the ALS and several user groups, provides an easy-to-use facility to perform soft x-ray absorption (XA) as well as x-ray magnetic circular dichroism (XMCD) measurements in external fields up to 2 T.

Mentoring and Pipeline for Future Scientists. Establishing a pipeline for future beamline and accelerator scientists is vital to all BES user facilities. Many Scientific Support Group members mentor students at all levels throughout the year. The Scientific Support



Doing AP-XPS on a working fuel cell.

Group has also established the ALS as a leader in setting up the pipeline for synchrotron scientists by establishing graduate student and postdoctoral fellowship programs. *http://www.als.lbl.gov/als/fellowships/.*

New Science. The following selection of highlights represent not only world-class science but also the unique capabilities created at the ALS by the Scientific Support Group: nanoparticle catalysis (see feature article); bandgap engineering with graphene [*Nature* **459**, 820 (2009)]; selective binding of alkali cations with carboxylate [*PNAS* **105**, 6809 (2008)]; chemical changes in cells under extreme conditions [*PNAS* **106**, 12599 (2009)]; iron pnictides [*Phys. Rev. B* **80**, 014508 (2009) and *Physics* **2**, 60 (2009)]; topological insulators [*Nat. Phys.* **5**, 398 (2009), *Science* **325**, 178 (2009), and over 100 press releases as well as coverage by ABC television]. ■

Crystallography

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Remote data collection has also risen significantly, and it now accounts for approximately 50% of all BCSB users. This increased adoption has been driven by the introduction of NX remote desktop technology, which provides the remote user with the full complement of sample visualization, sample manipulation, beamline control, data acquisition, and data analysis tools exactly as they would see them if they were stationed at the beamline. This enhanced remote operation capability is coupled with 24-hour onsite support by BCSB staff who are able to assist immediately with loading additional samples for remote users or troubleshoot any issues that might come up.

Another mode of access to the BCSB beamlines is via the Collaborative Crystallography program. Under this scheme, users do not only apply for beamtime via the general user program, but also for an expert crystallographer who will conduct the experiments and data reduction on behalf of the applicants. Depending on the users, structure solution, model building, and refinement can be carried out as well. The collaborative crystallography program is utilized by a variety of academic user groups from across the globe, notably by groups involved in high-throughput, structural genomics efforts.

Improvements continue to be made to the optics and performance of all the BCSB beamlines. In Sector 5, the upgrades to the 5.0.1 and 5.0.3 monochromators have now been completed. The new monochromators increase the operational energy of both beamlines, taking them above the Se K-edge and thus introducing a significant new Se SAD capability for experiments on Se derivatized proteins. The new monochromators also provide significantly better beam focus and performance under the increased power loads of ALS top-off operation. These improvements have been coupled with the introduction of enhanced positional feedback, diagnostic tools, and auto-alignment systems for the beamline components to improve the overall stability and quality of the beam delivered to users. ■

PEOPLE AND EVENTS

A Good Year for Renewing the ALS

by Roger Falcone

I am pleased to report that the ALS has had a terrific year. We are seeing a positive growth slope in a number of areas, including funding, facilities, and safety. With our Strategic Plan already in place at the end of last year, we were in an excellent position to capitalize on opportunities to launch new initiatives. In addition, growth in FY09 and (proposed) FY10 budgets indicates that new projects will proceed. The ALS also successfully transitioned to top-off mode in February, a critical upgrade that has resulted in twice as much light as before, as well as more stable and reliable operation.

In 2009, we underwent a major DOE Health, Safety, and Security (HSS) review, from which we emerged with the top rating given, the only light source nationally and the only Berkeley Lab division to do so. The ALS response to the pending HSS review, under the leadership of Jim Floyd, was taken very seriously, and involved the entire ALS community, from management, to beamline scientists and users, to technical and administrative staff. The review concluded that all Integrated Safety Management core functions were "effectively performed." This is an extremely positive result because it 1) lets us know that, while we still have work to do, we're on the right track; 2) supports the contention that safety contributes positively to the mission of the ALS; and 3) allows the ALS to have a greater impact on broader safety policies and programs, as a model both within Berkeley Lab and throughout DOE.

Our base budget increased about 10% in FY09. In addition, we received supplemental funding in FY09, which will allow us to complete previously stalled projects and important maintenance work. Funds under the American Recovery and Investment Act allowed us to accelerate construction of the User Support Building and purchase new air-handling units for the ALS. We are also pleased that $11.3M in Recovery Act funds were awarded for four major projects: sextupole magnets, a high-field magnetometer, an EPU for Sector 6, and cutting-edge detectors. A further $2.5M has been allocated for R&D on advanced detectors and a next-generation soft x-ray free-electron laser source. In addition, we received a $4.4M grant for nanoARPES at the new MAESTRO beamline in Sector 7.

With all these developments, plus light at the MERLIN beamline, the pending opening of the Guest House, and new faces showing up around the ALS, it has truly been a landmark year and I'm looking forward to another, thanks to the efforts of the entire ALS community! ■

Users' Executive Committee Update

by Kenneth A. Goldberg, 2009 UEC Chair

It is my pleasure to serve as the 2009 UEC Chairman. Each year, more that 2,000 researchers use the ALS's 30-plus beamlines in their research. The ALS management and staff deserve tremendous credit for managing the complex flow of scientists, samples, and safety rules so productively. Whenever their decision-making and strategic planning can benefit from the direct input of ALS users, they turn to the Users' Executive Committee (ALS UEC) for input. In an open, continuous, two-way exchange, the eleven elected members of the ALS UEC represent the user community to the management. Working at the ALS, and being involved with the UEC, I find that there is never a lull in ALS activities. 2009 has been a tremendous year, with unexpected opportunities, and with the results of our hard work paying dividends.

The flurry of preparation surrounding the Health Safety and Security (HSS) audit resulted for many of us in a much clearer conception of what is required of users, staff, and beamline scientists, as we plan and conduct our daily work. The ALS's emergence from the audit with a high score in every category, ahead of all other reviewed divisions within Berkley Lab, could only have happened with the close coordination the management, staff, and users, and with the high degree of professionalism and dedication that those of us who work here often take for granted. With some persistently challenging safety issues (such as food policy and the necessity of safety glasses on the experiment floor), frequent consultations with the UEC and feedback from a poll of users provided useful input that helped the ALS reach agreement with Berkeley Lab management on workable new safety rules that we can all live with.

On the building front, our temporary parking frustrations are a small price to pay for rapid progress on new facilities serving the ALS community. The new User Support Building is coming together quickly, and the Berkeley Lab Guest House will be open by the time of the ALS Users' Meeting. These are facilities that the ALS users have supported for many years.

The most visible role of the UEC, and the highlight of our year, is the annual ALS Users' Meeting, which is being held jointly with The Molecular Foundry this year. The ALS meeting program co-chairs, Yayoi Takamura and David Osborn, with the help of Sue Bailey and her team at the ALS User Services Office, have put together an outstanding program for the 2009 meeting. We hope our joint activities with the The Molecular Foundry lead to the fruitful cross-pollination of ideas in materials synthesis and analysis.

Finally, I would like to thank the members of the ALS user community for your support and help. I encourage every user to become involved with the UEC—run for office! It is your chance to give back, to advocate for the great work that goes on here, and to help ensure that the ALS's best years are still to come.

I wish you all an enjoyable, exciting, and productive future at ALS. ■

PEOPLE AND EVENTS

Meet Our New Deputy Director for Science: Bob Schoenlein

In March, it was announced that Robert (Bob) Schoenlein would join the ALS as Deputy Director for Science. Bob's research is in the area of ultrafast science, with programs in Berkeley Lab's Materials Sciences and Chemical Sciences Divisions (MSD and CSD, respectively). His involvement with the ALS dates back more than 15 years, beginning as a somewhat unconventional "ALS user"—first joining with an interdisciplinary team of colleagues from the Lab's Accelerator and Fusion Research Division (AFRD) and the ALS to develop laser-based techniques for manipulating electron beams to generate ultrafast x-rays, and then applying these unique sources to studies of structural dynamics in matter.

In the mid 1990s, Schoenlein, W. Leemans, and colleagues used Thomson scattering with the ALS linac injector to generate femtosecond hard x-ray pulses for some of the earliest subpicosecond diffraction studies. Even newer ideas from AFRD colleagues A. Zholents and M. Zolotorev, based on injecting femtosecond laser pulses into the storage ring, were demonstrated on Beamline 6.3.2 and further developed at the prototype femtosecond x-ray Beamline 5.3.1 with ALS Scientists P. Heimann and E. Glover. This approach is the basis for the new Ultrafast Slicing Beamlines 6.0.1 and 6.0.2, which support Bob's current research (on dynamics in complex materials and condensed-phase molecular dynamics) as well as that of many other ALS users in the growing field of ultrafast x-ray science.

In addition to his new role as Deputy Director for Science, Bob plans to remain active as a researcher within MSD, CSD, and at the ALS. Of course his first priority will be to support the world-class science program of the ALS, which he believes is a testament to the outstanding scientific staff, technical staff, and user community of the ALS. His major goals are to maintain and build on this record of excellence—fostering the development of new research directions and exploiting new scientific opportunities. He is looking forward to working closely with ALS scientific staff, users, and advisory committees to meet these challenges and to helping Roger and his team implement the ALS Strategic Plan that will serve as a roadmap for the facility into the next decade and beyond. Bob is fortunate to have the opportunity to work with ALS Science Advisor and former Director Janos Kirz during a transition period. This leaves only one grand challenge standing between Janos and retirement from management responsibilities—passing along his extensive knowledge, expertise, and scientific judgment that has served the ALS so well. ■

Positive Report from DOE Health, Safety, and Security Audit

by Jim Floyd

As you all know, ALS was one of the divisions selected for the recently concluded Department of Energy (DOE) Health, Safety, and Security (HSS) audit. This was the most comprehensive safety inspection Berkeley Lab has undergone in more than a decade. At the ALS alone, more than 40 people were observed performing work, auditors sat in on several of our safety meetings, and dozens of documents were reviewed during the three weeks that they were here.

We are very happy to report that HSS found all of our Integrated Safety Management (ISM) Core Functions to be "effectively performed," the top rating. This is an extremely positive result for our division and we should be very proud of this accomplishment. We think we've all come to realize the importance of safety, both as an ethical and legal imperative, and for its impact to our scientific mission. Safety is now an important part of generating confidence on the part of our funders so reports such as this play a big role in our ability to continue to succeed.

One comment in the report is especially meaningful: "Division management and staff displayed their commitment to teamwork and safety in the development and implementation of hazard controls...." We know how hard all of you have worked this last year and we have seen your dedication and teamwork, so it is very gratifying to see that this was also recognized by HSS. Your openness and willingness to learn from this review went a long way towards achieving this measure of recognition.

However, we should recognize that we still have many areas that we can and need to improve upon. The appendices to the report list many items that they found during their time here and we all identified many more as a result of this process. This report, however, clearly shows that we've accomplished much and are on the right track. Many thanks again to all of you. ■

PEOPLE AND EVENTS

ALS Attracts High-Profile Visitors

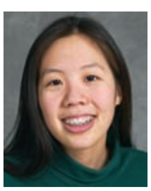
The ALS remains a must-see stop for visitors to Berkeley Lab, including high-profile dignitaries from federal, state, and local government.

On a West Coast trip in late June, Department of Energy (DOE) Secretary Stephen Chu visited Berkeley Lab, where he served as Director from 2004 through 2008. While here, Chu attended a small reception and heard presentations on a variety of research projects underway at the Lab, from carbon dioxide fixation to hydrogen storage to graphene breakthroughs, the latter given by the ALS's own Eli Rotenberg. Also in attendance were Berkeley Lab Interim Director Paul Alivisatos, Lab Chief Operating Officer Jim Krupnick, ALS Division Director Roger Falcone, and Physical Biosciences Acting Division Director Paul Adams. DOE Deputy Secretary Daniel Poneman also visited the Lab, on August 19. In addition to the ALS, his tours included the Joint BioEnergy Institute (JBEI) and the Molecular Foundry. He also listened to presentations on the Lab's strategic initiatives and solar-to-fuels and climate change research. Kristina Johnson, DOE Under Secretary for Energy, visited Berkeley Lab on June 22 for meetings with scientists and tours of laboratories and national user facilities, including the ALS. In addition to learning about the Lab's energy efficiency and renewable energy research initiatives, Johnson toured the Old Town site and learned about the need for infrastructure modernization at the Lab.

Reception for DOE Secretary Steven Chu (far left) at Berkeley Lab; ALS Director Roger Falcone is on the far right.

South Dakota Governor Mike Rounds toured the ALS as part of a visit on June 12. He came to Berkeley Lab to get a feel for the type of research operation that will be built at his state's Homestake gold mine. The Deep Underground Science and Engineering Lab (DUSEL) will host experiments in a *continued on page 15*

Honors and Awards



Sakdinawat

At the International X-Ray Microscopy meeting (XRM 2008) in Zurich, Switzerland, Anne Sakdinawat was presented with the prestigious Werner Meyer-Ilse Award (along with co-recipient Pierre Thibault of the Paul Scherrer Institute). The award is presented every third year for contributions to the development of x-ray microscopy. Anne was honored "for the development of modified zone plates for phase contrast and high depth of focus applications." She received her Ph.D. from the University of California, Berkeley, Department of Bioengineering; has been at Berkeley Lab's Center for X-Ray Optics (CXRO) for the past five years; and is also a member of the ALS Users' Executive Committee (UEC). Her research was performed at ALS Beamlines 6.1.2 and 12.0.2.

Rotenberg

Eli Rotenberg, Deputy Leader of the ALS Scientific Support Group, has been elected a Fellow of the American Physical Society (APS). His citation reads: "For outstanding contributions to the understanding of quantum electronic properties of nanophase and reduced dimensionality systems by creative applications of angle-resolved photoemission spectroscopy." Election to Fellowship in the APS is limited to no more than one half of one percent of the membership, and is recognition by peers of outstanding contributions to physics.

Saykally

Long-time ALS user and Berkeley Lab chemical scientist Richard Saykally has received the Peter Debye Award in Physical Chemistry, bestowed by the American Chemical Society. Laser spectroscopy of liquids, surfaces, and clusters; synchrotron x-ray spectroscopy of liquids and liquid surfaces; and femtosecond nonlinear optical spectroscopy of liquid surfaces are among the areas in which Saykally conducts research. Peter Debye, the award's namesake, was a Dutch physicist and physical chemist, and Nobel laureate who died in 1966.

Fadley

Chuck Fadley, a scientist with the Materials Sciences Division and a veteran researcher at the Advanced Light Source where he has gained recognition as one of the world's foremost practitioners of photoelectron spectroscopy, has been unanimously elected as a "Foreign Member" of the prestigious Royal Society of Sciences in Uppsala, the oldest learned society in Sweden. In recent years, Fadley has led the development of techniques for studying nanolayers of materials that shed new light on such important phenomena as colossal magnetoresistance and high-temperature superconductivity. ■

Beamline 11.0.2

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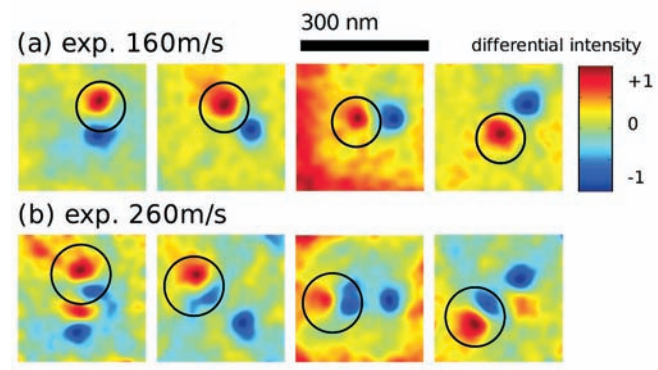
versus the solid phase (due to increased solubility in the solution phase) and the polarizability Br^- in the solution.

In recent years, experiments using the STXM at 11.0.2 have provided a number of groundbreaking experiments in magnetic materials. One such study focused on the core reversal mechanism of magnetic vortices. Magnetic nanostructures that exhibit a magnetic vortex state have a core where the magnetization can point either up or down. The vortex core has a diameter of only 5 to 20 nm and is difficult to observe, its dynamic behavior in particular. STXM was used to elucidate the first step of a core-reversal process: the dynamic deformation of the vortex core. These studies provided the first experimental support for the theoretical predictions of the creation and annihilation of a vortex–antivortex pair.

Over the last year, a wide range of improvements were continually undertaken to advance the scientific capabilities of this beamline. These include the continued development of a mini-STXM for vacuum magnetic experiments and a droplet train apparatus for experiments in aerosol chemistry. ■



(a) Differential STXM images under a continuous 0.32 mT radiofrequency excitation. Red corresponds to the magnetization pointing up, and blue corresponds to down. The vortex core is seen as a red spot, indicated by the black circle. (b) Images of the same sample, but with a 0.89 mT excitation. The dynamic vortex core deformation is now visible as an extra spot near the vortex core [Vansteenkiste et al., *Nat. Phys.* 5, 3332 (2009)].

CXRO

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within the frame of an analytical model and revealed the velocity and mass of the DW. A stochastic character of the DW depinning process in magnetic nanowires was found, which also has implications for technological devices, but can be controlled by selecting a proper wire geometry. Figure (b) shows x-ray images of field-driven DW propagation in such nanowires.

The Sematech Micro Exposure Tool (MET) on Beamline 12.0.1.3 provides the world's highest-resolution EUV print capability for evaluating resist materials and mask research. Resist innovations are pushing the envelope of resolution (20-nm half-pitch lines), sensitivity, and line-edge roughness. Figure (c) shows the cross section of an EUV resist at 22-nm resolution. The MET has also been used to uncover subtle mask effects contributing to line-edge roughness. This work is now leading to industry discussions on developing new mask standards. Also used for EUV mask research is the EUV zone-plate aerial imaging tool (AIT) on Beamline 11.3.2 that emulates the optical parameters of EUV lithography systems. As the highest-performing tool of its kind, it serves a broad group of semiconductor company researchers by finding and classifying mask defects as small as 20 nm wide and 1 nm tall and by validating the effectiveness of repair and cleaning strategies. ■

High-Profile Visitors

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range of fields, including physics, earth sciences, biology and engineering. Doug Clapp, a representative of the Senate Energy and Water Development Appropriations Subcommittee, visited the Lab on May 28. Clapp toured the ALS, JBEI, the National Center for Electron Microscopy, and the Molecular Foundry, among other locations. He received briefings on next-generation light source plans, solar-to-fuels and batteries, computing, the Joint Dark Energy Mission, and DUSEL.

On July 15, members of the University of California (UC) President's Associates visited Berkeley Lab for briefings on biosciences work at the Lab. The President's Associates include the spouses of UC Chancellors and Mrs. Judy Yudof, wife of UC President Mark Yudof. Roger Falcone welcomed the group and gave them an overview of the diverse research capabilities of the ALS. Beamline scientist Corie Ralston followed with a short presentation on structural biology research at the ALS with implications for diseases such as Alzheimer's and autism. Also, as part of a regular meeting with Lab leadership, Berkeley Mayor Tom Bates toured the ALS and the Old Town area just up the hill. He also met with Berkeley High teachers and students who are participating in internships at the Lab this summer. Discussion topics also included Lab construction and truck traffic, the East Bay Green Corridor program, and possible collaboration on projects funded by the American Recovery and Reinvestment Act. ■

FACILITY UPDATES

Accelerator Availability and Reliability

by David Robin

The ALS operating schedule is divided into user beam shifts, accelerator physics/machine setup shifts, maintenance and installation, and vacation shutdown shifts. In a "typical year," there is usually one long shutdown for major servicing, large installations, and upgrades. This long shutdown and associated startup usually occurs in the spring and lasts about six weeks. Also, in a typical year the ALS schedules and delivers more than 5000 beam hours to users. Below is a summary of events during the previous three fiscal years and the availability and reliability of the facility.

Availability is one of the most important performance parameters of the facility. Availability is defined as the ratio of delivered versus scheduled user time, while reliability is defined as the ratio of the number of actual fills that were completed without interruption versus the number of scheduled fills. Maintaining a high availability as the facility becomes more mature and complex (e.g., the addition of new insertion devices, injector upgrades, feedback and feed forward) is a challenging task.

The number of hours scheduled and delivered is shown in the table. In this review period, there was a deviation from the typical yearly shutdown pattern as described above. In FY06 the ALS ran the entire year without a major shutdown, and in FY07 the ALS had two long-term shutdowns—one in the fall of 2006 and the other in the spring of 2007. Therefore, the number of scheduled and delivered user hours were rather different in those two years. Because of this anomaly, it is convenient to look at the availability over the entire three years. Of the 16,001 scheduled hours, the ALS delivered 16,602 hours, which averages to 5534 hours per year, with a total availability of 94.6% delivered in schedule.

There was a drop in availability in FY07 and a partial recovery in FY08. This was because of two cascading effects that arose from the injector upgrade. In the fall of 2006, the ALS underwent a major shutdown to install and commission components necessary for full-energy injection. At the end of the shutdown, there was a major failure in one of the components (the booster bend power supply), which resulted in a loss of nine user days. The second effect was that this failure resulted in longer fill times for the remainder of FY07 and FY08.

Reliability is another important performance parameter of the facility, which is distinct from availability. Reliability is defined as the ratio of the number of actual fills that were completed without interruption versus the number of scheduled fills. Providing good availability is necessary but not sufficient to ensure good reliability. For example, a user run with many unscheduled dropouts but fast recovery times would result in good availability but poor reliability. A good measure of reliability is the mean time between failures (MTBF). The MTBF was 50 hours in FY06, 51 hours in FY07, and 46 hours in FY08. The reduced reliability has largely been due to growing pains associated with top-off, and indications are that we will see improvements in these numbers in the near future. ■

HOURS SCHEDULED AND DELIVERED

	Scheduled hours	Delivered hours*	Availability	Mean time between failures (hours)
FY06	6201	6045	97.5%	50
FY07	4200	3864	92.0%	51
FY08	5000	4664	93.0%	46

*Does not include unscheduled hours delivered to users.

User Demographics and Publications

by Sue Bailey

As a national user facility, the ALS is required to report user demographics and publication information annually to the U.S. Department of Energy. Figure 1 shows the breakdown of different types of institutions that make up our user base. The overall user growth and the growth in particular scientific fields from 1998–2008 is shown in Figure 2. The overall number of users at the ALS has stabilized at around 2000 following the effects of two shutdowns that occurred in FY07. The exact numbers are highly correlated with the number of shifts of beamtime supplied to users in a given year. As the number of beamlines approaches the capacity of the storage ring, new beamlines will be created by chicaning straight sections and revamping some of the older bend-magnet beamlines. The scientific productivity of the ALS as measured in refereed and high-profile publications since 1994 is shown in Figure 3. ■

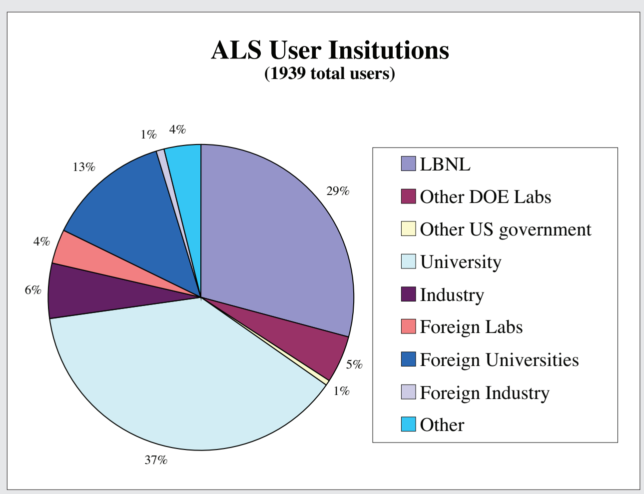

Figure 1. Pie chart showing percentages of different types of user institutions.

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FACILITY UPDATES

Construction Projects Update

by Steve Rossi

The User Support Building (USB) project has faced many funding challenges, but thankfully those days are now behind us. The project received its scheduled FY09 funding of $11.5M and was also forward funded its scheduled FY10 funding of $14.5M under the American Recovery and Reinvestment Act (ARRA). With all of the project's $35M budget in hand, construction activities can now proceed uninterrupted and be completed in the most efficient way possible. It is worth noting that the ARRA funds will allow the project to be completed three months early and will also save the project approximately $500k, which will in turn be used to better the project.

In July, the project met an important construction milestone when the structural steel was completed. August and September construction activities focused on the installation of mechanical, electrical, and plumbing utilities as well as interior and exterior stud walls. Construction is proceeding on schedule, which should allow us to take occupancy of the building in August or September 2010.

The Berkley Lab Guest House is now complete and open for business. Located within a short walk of the ALS and the cafeteria, the 57-room Guest House provides 70 beds in single- and double-occupancy rooms, and includes a main lobby, lounge/kitchenette area, laundry facilities, vending areas, and an outdoor patio. All rooms have a refrigerator and free wireless Internet access.

I think you will find the Guest House very comfortable and that it uniquely meets your needs since the facility was designed with you, the ALS user and visitor, in mind. In addition to the features above there were many things done in the construction and fit-up process to make you comfortable such as the inclusion of operable windows, very quiet locally controlled in-room heat/air conditioning, sound dampening between floors and on piping, black-out window shades, and high-quality mattresses and linens. Rates start at $119 per night and are not subject to any local or state taxes. Please visit *http://berkeleyscience.org/ berkeleylabguesthouse/* for more information and to make reservations. ■

Updated rendering of the User Support Building.

Guest House construction as of September 1, 2009.

User Demographics and Publications

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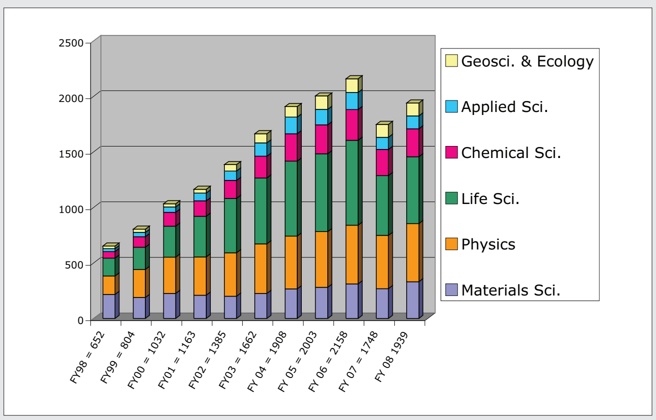


Figure 2. Bar graph showing growth in various areas of science. The 2007 numbers reflect the two shutdowns that occurred in FY07.

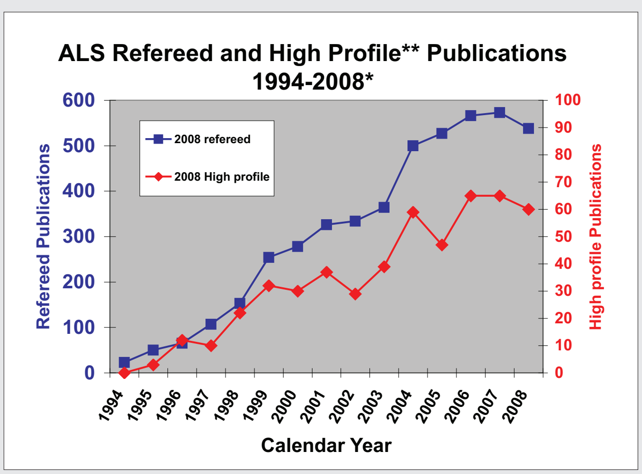


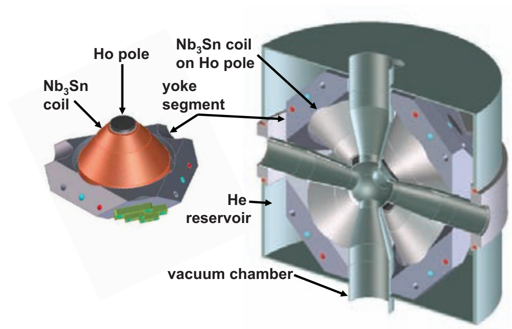
Figure 3. Graph of growth in refereed publications (blue) and high-profile publications (red). *Note that publications for 2008 were still being collected at the time this section was being written. **High-profile publications include Nature, Science, PRL, and Cell.

FACILITY UPDATES

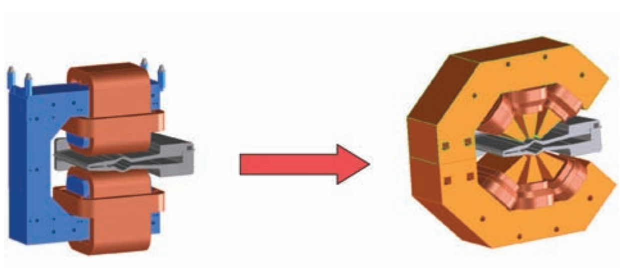
ALS Gets $11.3 M in Stimulus Funds for Facility Improvements

The ALS is receiving $11.3 million to help it maintain its position as one of the world's premier soft x-ray light sources. Four items from the ALS strategic plan have been approved for funding though the American Recovery and Reinvestment Act (ARRA).

First, the ALS will receive $5.8 million to increase brightness by replacing existing corrector magnets with hybrid multifunction sextupole magnets. This lattice upgrade would increase brightness by a factor of three in the center-bend-magnet beamlines and up to a factor of two in the insertion-device straights. Second, the ALS will receive $2 million to construct and install an elliptically polarizing undulator for the femtosecond soft x-ray Beamline 6.0.2, effectively doubling its capacity by enabling soft and hard x-ray branchlines to operate simultaneously. Third, the ALS will receive $2 million to equip beamlines with advanced CCD-based detectors developed at Berkeley Lab. These detectors, which are well beyond the commercially available state of the art, will dramatically increase the reach and scientific productivity of each of the beamlines where they are deployed. Fourth, the ALS will receive $1.5 million to develop a superconducting vector magnetometer with a magnetic field of over 5 Tesla in any orientation relative to the sample and photon polarization. The high magnetic field will allow experiments leading to novel insights into the magnetic structure of engineered magnetic nanostructures and materials not accessible by any other technique.



Design sketch of the superconducting eight-pole magnet generating magnetic fields of up to 6 T in arbitrary directions for soft x-ray magnetic dichroism experiments at ALS.



Replacing existing corrector magnets with hybrid corrector/sextupole/skew elements.

It is estimated that the funding will create the equivalent of more than 19 jobs at the Lab and 65 jobs externally.

Beyond the items described above, several ALS-related infrastructure projects will also receive ARRA funds. The ALS User Support Building, currently under construction, has been forwarded $14.6 million for FY10 funding. The project, which has had funding challenges in the past, can now proceed uninterrupted and be completed in the most efficient way possible. Building 6, which houses the ALS experiment floor as well as offices, labs, and conference rooms, will receive $1.5 million to replace three aging air handling units that had some vibration issues, negatively impacting scientific studies, with higher-capacity and higher-efficiency units. Building 2, which provides office, laboratory, and conference-room space adjacent to the ALS, will receive $2.9 million for upgrades to its cooling system.

Visit *http://recovery.lbl.gov* for more details on all Berkeley Lab's ARRA projects. ■

Science Roundup

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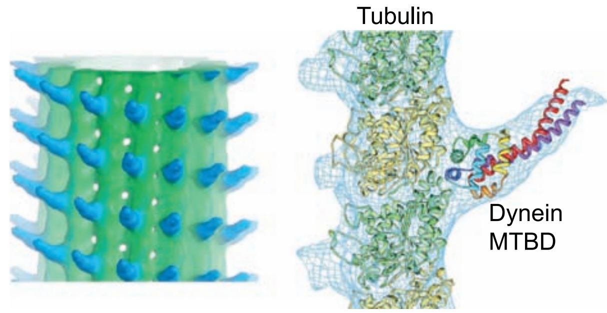
sity who studied the electronic structure of insulating alloys of bismuth and antimony by means of angle-resolved photoemission spectroscopy (ARPES) and spin-resolved ARPES. Their results constitute the first direct experimental evidence of a topological insulator in nature that is fully quantum entangled. In the future, a detailed study of topological order and quantum entanglement using their method can potentially pave the way for fault-tolerant (topological) quantum computing.

How Dynein Binds to Microtubules

Carter et al., *Science* **322**, 1691 (2009)

http://www.als.lbl.gov/als/science/sci_archive/185dynein.html

Cytoplasmic dynein is a protein complex responsible for the transport of a large variety of cargoes, from specific RNAs and proteins to whole organelles, in a directional fashion along microtubules that serve as cellular conveyor belts. Consistent with this central role, cytoplasmic dynein is associated with a number of disease-related processes, including the transport of viruses, neurodegeneration, and the mitotic checkpoint malfunctions that lead to cancer. A team of researchers from the University of California's San Francisco and Berkeley campuses has recently solved the structure of dynein's microtubule-binding domain (MTBD) and part of the stalk structure that connects MTBD to the rest of the dynein complex. This first look at any part of the dynein motor domain identifies how it binds to microtubules and gives some hints into the fascinating question of how communication passes along the stalk from the MTBD to the rest of the motor. ■



Left: Cryoelectron microscope image of dynein MTBDs (blue) bound to a microtubule (green). Right: MTBD and tubulin structures docked into an electron-density map (blue mesh) of a single microtubule protofilament decorated with dynein MTBDs.

Experimental Systems Group

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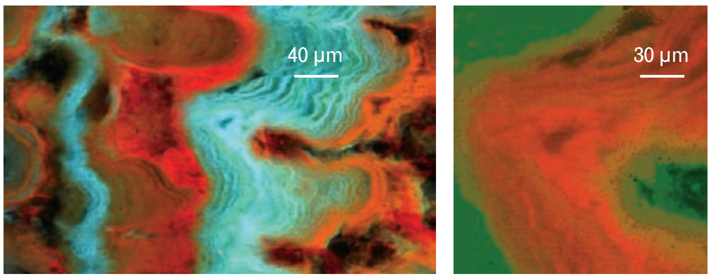
to the region is required. For this we implemented in the beamline control system a fast XRF scan module that can be correlated with visible images extracted from either the viewing system or from separate SEM experiments. New methodologies were also introduced, such as energy-resolved Laue diffraction allowing use of Laue spot intensity information for crystal structure refinement and exploitation of monochromatic "powder" patterns for triaxial strain measurements.

At Beamline 10.3.2, our hard x-ray micro-XRF/XAS/XRD line, the focusing mirrors were replaced, taking the minimum spot size down to ~1 µm from 3–4 µm and eliminating low-energy scattering tails. These new-generation K-B mirrors were developed in-house and are bendable to achieve a near-perfect elliptical shape. The mirrors are first adjusted using optical methods in our metrology lab, and the final shape is achieved in situ. The method currently used on all our x-ray microfocus lines is based on the Hartman method, whereby a slit before the mirrors defines a collimated x-ray source, focused to the image plane. Moving the slit perpendicular to the beam results in a very small amount of image motion, sensed with a repetitively scanned knife edge. This motion is analyzed in real time, and corrections are made to the two bending couples applied to each mirror. In this way, resolution can be optimized before experiments.

As the source brightness improves, it creates a greater need to improve beamline optics, using the types of automated methodologies described above. It also puts a greater emphasis on using the best detector technologies available, such as commercial pixel detectors, and on new in-house designed energy sensitive x-ray CCDs. Like the storage ring, which over the last 15 years has improved in brightness by a factor of 100, similar or even larger gains can be made with relatively modest investments in beamlines and endstations. With these improvements, we can look forward to a bright future! ■



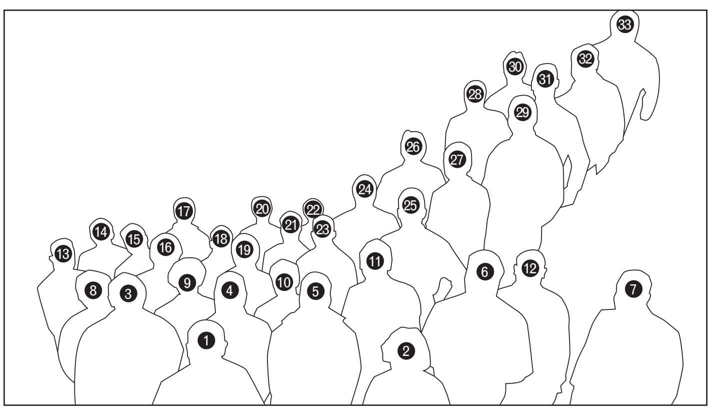
A deep-ocean ferromanganese nodule imaged in Fe (red), Mn (green), and Cu (blue) at 0.8-µm pixel using the new optical system of Beamline 10.3.2 [B. Toner (U. of Minnesota), K. Edwards and G. Horn (Woods Hole Oceanographic Institution), S. D'Hondt (U. of Rhode Island)].

Top-Off Success

continued from page 4

of three. Another example was the development of simulation methods for the top-off safety analysis, which required the creation of new computer codes.

Many thanks and congratulations to the top-off project team, lead by David Robin and Christoph Steier, as well as many other people from the ALS, engineering, accelerator operations, and EH&S staff who helped to make this upgrade a success. ■



Top-off team members: (1) Ron Gervasoni, (2) Helen Chen, (3) Mike Fahmie, (4) Ken Baptiste, (5) Walter Barry, (6) Bill Kelius, (7) Fernando Sannibale, (8) Jin-Young Jung, (9) Alexis Smith-Baumann, (10) Alex Gavidia, (11) Hiroshi Nishimura, (12) Max Vinco, (13) Bill Kenney, (14) Barry Bailey, (15) Steve Cooper, (16) Christoph Steier, (17) Greg Portmann, (18) Tony Warwick, (19) Weishi Wan, (20) Chris Hernikl, (21) Steve Rossi, (22) Ryan Sprague, (23) Pat McKean, (24) Tom Scarvie, (25) Mike Kritscher, (26) Warren Byrne, (27) Mike Chin, (28) Jonathan Elkins, (29) David Robin, (30) Pat Casey, (31) Jonah Weber, (32) Moises Balagot, (33) Bob Mueller. Not pictured: Alan Biocca, Richard Donahue, James Dougherty, Bill Gath, Susanna Jacobson, James John Julian, Slawomir Kwiatkowski, Steve Marks, Jim Oneill, Ross Schlueter, Derek Shuman, Greg Stover, Chris Timossi, Eric Williams, Russell Wells.

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